

University of Groningen

## Conformational Changes in the Bacterial Translocase Subunit SecA

Blaauwen, T. den; Driessen, A.J.M.

**IMPORTANT NOTE:** You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

*Document Version*

Publisher's PDF, also known as Version of record

*Publication date:*

1996

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Blaauwen, T. D., & Driessen, A. J. M. (1996). *Conformational Changes in the Bacterial Translocase Subunit SecA*.

### Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

### Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

### A3 Structural dynamics

P-A3-01

#### MOLECULAR DYNAMICAL THEORY FOR SPONTANEOUS EMISSION OF BIO - PHOTONS IN THE LIVING SYSTEMS DANG XIAO - FENG

Dept. of physics, Southwest Institute for Nationalities, Chengdu 610041, and Institute of Atomic and Molecular physics, Sichuan Union University, Chengdu 610065, China

**Purpose:** Many experiments show that the bio - photon emission including thermal radiation and  $\gamma$  - photons of the Living systems is a general and important biological phenomenon. We propose here a theory of molecular biology for the emission of bio - photons.

**Methods:** We think that the bio - photon emission come from the transition of bonding electrons and displacement of active nuclei and non - linear vibration of molecular chains resulting from the solitons excited by the intramolecular localized fluctuation and the deformation of structure and conformation of molecular chains caused by the energy released in ATP hydrolysis in biomacromolecules with biological temperature. The Hamiltonian and Wave function in our theory are

$$H = \sum_i \left[ \frac{1}{2m} p_i^2 + \frac{m}{2} \omega_i^2 q_i^2 - \frac{m\omega_i^2}{2} q_i q_{i+1} \right] + \sum_i \left[ \frac{M}{2} R_i^2 + \frac{1}{2} \lambda (R_i - R_{i-1})^2 - \frac{\lambda}{3} (R_i - R_{i-1})^3 \right] + \sum_i \left[ \frac{m\lambda}{2} (R_{i+1} - R_i)^2 + m\lambda (R_{i+1} - R_i) q_{i+1} \right],$$

$$|\Phi\rangle = \frac{1}{\lambda} \sum_i (1 + q_i(t) b_i^\dagger) \exp \left[ \sum_i (a_{q_i}(t) a_{q_i}^\dagger - a_{q_i}^\dagger(t) a_{q_i}) \right] \pi \left( \frac{a_{q_i}^\dagger}{\sqrt{q_i}} \right) |0\rangle$$

**Results:** applying non - linear quantum theory we find out the Intensity of bio - photon emission to be

$$W = \frac{256\alpha_0^2 \hbar^2 \omega^2}{9M^2 V_0^2 \omega^2 (\hbar^2 \omega^2 - \hbar^2 \omega_0^2)} \left[ -\vec{M}(\vec{x})_1 \cdot \vec{x} - \vec{M}(\vec{x})_2 \cdot \vec{x} \right] \sin^2((\omega_0 - \omega)t/2) / (\omega_0 - \omega)^2 \left[ [A^2(T) \cos^2(\vec{E} \cdot \vec{h}) + (v(t - x_0))] \right] \frac{\vec{E}^2 \cosh^2(1)}{2\omega(\vec{E}^2 + 1)} + A^4(T) \frac{\vec{E} \cdot \vec{h}}{\omega} \sin^2(\vec{E} \cdot \vec{h}) + (v(t - x_0)) \exp \left[ - \sum_i \frac{(\vec{E} \cdot \vec{e}_i)^2}{2M\hbar\omega_i} \cosh \left( \frac{\hbar V_i \cdot \vec{q}}{2K_B T} \right) \right]$$

**Conclusions:** with the help of this result, we can explain all phenomena and properties of bio - photon emission obtained from experiments.

P-A3-03

#### PHOTOSENSING IN EUBACTERIA: TRANS/CIS ISOMERIZATION OF THE CHROMOPHORE OF PYP

KORT, R., CRIELAARD, W. AND HELLINGWERF, K.J.

E.C. Slater Institute, University of Amsterdam (NL)

**Purpose:** Photoactive yellow protein (PYP) is a cytosolic eubacterial blue-light photosensor with a rhodopsin-like photocycle. The photochemical basis of the photocycle of PYP has been investigated to find a rationale for the high similarity of its photocycle to that of sensory rhodopsins, in spite of great structural differences.

**Methods:** The *p*-coumaric acid chromophore was extracted from the ground state of PYP (pG) as well as from the blue-shifted photocycle intermediate (pB). Extracts were analyzed by zone capillary electrophoresis and <sup>1</sup>H-NMR spectroscopy.

**Results:** Analysis of the chromophore extracts from pG and pB demonstrated that the chromophoric group of PYP isomerizes from *trans* to *cis* *p*-coumaric acid while progressing through the photocycle.

**Conclusions:** These results contribute to the understanding of the similarity in photocycle between PYP and sensory rhodopsins and show that also in Bacteria, so in all three domains of life, photosensing occurs by a common photochemical basis: isomerization of a chromophore double bond.

P-A3-02

#### CONFORMATIONAL CHANGES IN THE BACTERIAL TRANSLOCASE SUBUNIT SECA

DEN BLAAUWEN T., DRIESSEN A.J.M.

Groningen Biomol. Sci. and Biotech. Institute, Univ. of Groningen (NL)

The homodimeric SecA protein is the peripheral subunit of the preprotein *translocase* in bacteria. It binds the preprotein and promotes its translocation across the bacterial cytoplasmic membrane by nucleotide modulated co-insertion and de-insertion into the membrane. SecA has a high affinity nucleotide binding site (NBS-I) in its amino terminal domain and a low affinity NBS (II) in its carboxy-terminal domain. The conformations of the nucleotide bound states of SecA were studied by site directed tryptophan fluorescence spectroscopy, tryptic digestion, differential scanning calorimetry and dynamic light scattering. SecA unfolds as a two domain protein. ADP binding to NBS-I increases the interaction between these domains, whereas the non-hydrolysable ATP analog AMP-PNP does not influence this interaction. ADP binding to both sites induces a more compact state, which is thought to resemble the membrane de-inserted state of SecA. AMP-PNP induces a more extended conformation, which could resemble the membrane inserted state.

P-A3-04

#### CONFORMATIONS OF PROLINE DIPEPTIDE STUDIED BY AB INITIO METHOD

KANG YK

Dept. of Chemistry, Chungbuk Natl. Univ. (Korea)

**Purpose:** The low-energy conformations of *trans*- and *cis*-Ac-Pro-NHMe with down and up puckerings are studied in order to investigate the preference of the puckering of pyrrolidine ring for the preceding imide bond.

**Methods:** All ab initio calculations were carried out using the Gaussian 90 and 92 molecular orbital packages. Full geometry optimizations were performed at the direct HF/SCF level with the 6-31G\*\* basis set. Single-point MP2 calculations were also performed on the optimized conformations with the same basis set.

**Results:** The intramolecularly hydrogen-bonded C7 conformer is found to be most preferred. The down puckering seems to be about 1.5 kcal/mol more stable than the up puckering at the HF/6-31G\*\* and MP2/6-31G\*\* levels. The optimized structural parameters are in general consistent with X-ray structures of peptides.

**Conclusions:** The preference and population for down and up puckered structures with the *trans* and *cis* imide bonds calculated here agree reasonably with the results obtained from the analysis of X-ray structures of proteins. The degree of puckering for each conformer is well described by puckering amplitudes.